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Quasi-2D Unsteady Flow Procedure for Real Fluids (Preprint)

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Details of the numerical solution techniques, including explicit, point-implicit, and fully implicit schemes, used in a new quasi two-dimensional procedure for the transient solution of real fluids in system lines and volumes are presented. The procedure is coupled with a real-fluid properties database so that both compressible and incompressible fluids may be considered using the same code. The procedure has been implemented in Matlab/Simulink® as well as Fortran95 to allow for application on a wide variety of computer platforms. The computational efficiency of the various numerical methods is discussed to aid in selection for specific applications. Results for the transient flows of gaseous nitrogen and water in a pipe are presented to demonstrate the capability of the current techniques and the unsteady flow physics that can occur in system lines.

Nomenclature

A	=	cross-sectional area
A_p	=	wetted area
a_r	=	relative acceleration between inertial and absolute frames of reference
CFL	=	Courant-Friedrichs-Lewi number
c	=	speed of sound
E	=	total energy = $\rho\,(e + u^2/2)$
e	=	internal energy
F	=	flux of mass, momentum, and energy
H	=	static enthalpy
i	=	cell index
k	=	temporal order of accuracy for ODE15s solution methodology
m, n	=	index variables
p	=	static pressure
$\dot{q}$	=	heat flux input
S	=	source vector
t	=	time
U	=	state vector
u	=	absolute velocity
u_r	=	relative velocity
V	=	fluid volume = $1/\rho$
x	=	distance along solution domain
ρ	=	fluid density
τ_w	=	shear force (friction)

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I. Introduction

THE simulation of unsteady flows of non-idealized fluids in system lines and volumes is of interest for a wide variety of applications and industries, including air-conditioning systems, water/steam/oil piping networks, refinery systems, gas-turbine secondary flow-path and cooling networks, and liquid rocket engine propellant lines. Several approaches for simulating the dynamic behavior of such fluid-transmission lines have been reported. The lumped-analysis approach treats a flow passage as a series of fluid control volumes that conserve mass and energy linked by flow resistance elements that compute the flow between the volumes[1]. While this approach does conserve momentum in a quasi-steady sense at the flow resistances, the unsteady momentum term in the governing equations is neglected. Although so-called "continuity" waves can be captured using this approach, neglecting these terms leads to an inability to capture true "dynamic" waves required for simulating such phenomenon as water-hammer and pressure surge[2]. Another approach utilizes the Method of Characteristics[3], which is a general method for solving particular types of differential equations. The governing equations for fluid flow are compatible with this method and it has been used for simulation of fluid transmission lines[4]. While the unsteady momentum terms are retained using this method, other problems, particularly at the boundaries of components, make it difficult to apply to a modular system-level simulation tool. Modal methods have also been used when solution in the frequency domain is possible[5]. This technique represents the pressure and velocity distributions in the flow domain as a sum of an infinite series of mode shapes, similar to a Fourier series solution. While this method does present an elegant and efficient method for simulating idealized flows (e.g. incompressible, inviscid, laminar, etc), the addition of turbulent flow, real-fluid properties, heat transfer and phase change complicate the application of the method and reduce its attractiveness.

Since unsteady phenomena such as wave dynamics play an important role in the operation and testing of systems that contain fluid lines, a method that captures these transient effects is required. The development of a quasi two-dimensional, unsteady, two-phase flow solver with heat transfer and real-fluid properties using standard finite-difference/control-volume solution methods has been the subject of the present effort. Such a solver is geared towards modeling the dynamic behavior of fluid-filled lines and passages (i.e. the solution domain is much larger in one spatial dimension than in the others) accounting for the effects of changing cross-sectional area. In addition, the solver must be suitable for use as a module in larger system-level transient simulations of hydraulic and pneumatic systems, so the solution method must be computationally efficient. The following sections describe the modeling approach, numerical methodologies and test cases that have been utilized during the development of this model. Results are then shown for transient pipe flow of both nitrogen and water as a demonstration of the numerical capability and fluid physics that can be captured with the current procedure.

II. Approach

The model developed here represents fluid lines and flow passages where the length of the domain is much larger than the hydraulic diameter of the domain as a quasi two-dimensional domain. For these types of components, flow separations and non-axial velocities are minimal, hence the quasi-2D assumption is valid. The solver is targeted to the commercial Simulink® dynamic simulation software package from the MathWorks for integration into a larger suite of modules developed for simulating various systems. Simulink® was selected since it offers a wide range of capabilities, over a dozen robust differential equation solvers, extensive documentation and technical support, a modern graphically-based modeling paradigm, an existing user community across many disciplines, and commercially-funded code development and maintenance. A Fortran95 code using more traditional solution methods is also being developed in parallel to provide test cases for the Simulink® module.

The solver is being developed to account for varying flow area, friction, losses due to bends, real-fluid and two-phase flow effects, gravity and acceleration, heat transfer, and the capability to produce unsteady and steady-state solutions. Fluid properties are obtained from the REFPROP fluid property database[6] available from the National Institute for Standards and Testing (NIST). This database utilizes state-of-the-art Equation of State models to fully describe "real fluid" properties over a wide range of thermodynamic conditions, including liquid, vapor, mixed phase and supercritical fluid regimes. Properties that completely define the fluid thermodynamic state, as well as transport properties, are available as a function of any two thermodynamic parameters. Validated fluid models for over 80 pure fluids and over 180 fluid mixtures are available in the database. The database is accessed through a suite of Fortran77 subroutines that were compiled into the codes and obtain fluid equation of state model parameters from external files provided with the database.

Friction and heat transfer are modeled as source terms in the governing equations. This approach allows the flow to be modeled as one-dimensional and facilitates the computational efficiency. Friction (i.e. viscous losses and losses due to bends and fittings) and heat transfer coefficients are obtained from suitable correlations between the

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flow variables and the source terms. The methodology for modeling two-phase flow will be included in the final paper.

III. Governing Equations

The governing equations consist of the quasi two-dimensional Euler equations with source terms for viscous effects and general acceleration in a non-inertial frame.

$$\frac{1}{V}\frac{\partial UV}{\partial t}+\left[\frac{\partial F}{\partial x}\right]=\frac{S}{V} \tag{1}$$

$$U=\begin{vmatrix}\rho\\ \rho u\\ E\end{vmatrix},\quad F=\begin{vmatrix}\rho u_r\\ (\rho u u_r+p)\\ \rho u_r H\end{vmatrix},\quad S=\begin{vmatrix}0\\ \dfrac{pV}{A}\dfrac{dA}{dx}-\rho V a_r-\tau_w dx A_p\\ \dfrac{\dot{q}}{V}-\tau_w u_r dx A_p\end{vmatrix} \tag{2}$$

where ρ is the density, u is the absolute velocity in the inertial frame, u_r is the relative velocity in the non-inertial frame, a_r is the gravitational and relative acceleration in the non-inertial frame, E is the total energy, p is the pressure, H is the stagnation enthalpy, V is the local cell volume, A is the local line cross-sectional area, dx is the cell line length, A_p is the perimeter area, τ_w is the wall shear stress. The wall shear stress can be written in terms of a friction factor, f, which is a function of the local Reynolds number and the wall surface roughness. For the viscous flow examples presented below, the Churchill correlation[7] was used to determine single-phase friction factors using the equation:

$$f=\left[\left(\frac{8}{\mathrm{Re}}\right)^{12}+\frac{1}{(A+B)^{3/2}}\right]^{1/12},\quad A=\left[2.457\ln\left(\frac{1}{(7/\mathrm{Re})^{0.9}+0.27(\varepsilon/D)}\right)\right]^{16},\quad B=\left(\frac{37{,}530}{\mathrm{Re}}\right)^{16} \tag{3}$$

where Re is the local Reynolds number based on diameter.

Closure between the pressure, density, and energy is performed with an equation of state for real fluids by using the NIST REFPROP suite of thermodynamic routines. This allows for the solution of compressible, incompressible, and two-phase flows.

IV. Numerical Methods

Equations (1) and (2) may be solved with a variety of numerical schemes that are second-order accurate in space and time for "steady" or transient flow. These schemes currently include implicit, point-implicit, and explicit time-marching procedures. Multiple-grid convergence acceleration may be used in steady-flow schemes as well as in the inner iteration of time-accurate point-implicit schemes to dramatically reduce the number of steady or inner iterations. Multiple numerical schemes have been developed in the current procedure to provide flexibility and robustness when solving different flow conditions.

A. Implicit

The fully implicit discretization of Eqs. (1) and (2) may be achieved by representing the primary variables contained in U at the new time step rather than at the current time step. This results in an N system of equations where N is the number of nodes in the line to be solved. The coefficients of the matrix which multiplies the primary variable column matrix can be written as a tri-diagonal system (for second order spatial accuracy). Solution of the system of equations can then be determined by finding the inverse of the coefficients matrix.

An alternative to solving the system fully coupled in terms of a block-tridiagonal system, Eqs. (1) and (2) may be solved iteratively in a sequential manner. The Matlab/Simulink solution procedure[8], ODE15s, treats the discretized

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form of Eqs. (1) and (2) as a sequential set of ordinary differential equations and solves them iteratively with a Newton iteration according to the update formula:

$$\sum_{m=1}^{k} \frac{1}{m} \nabla^m U_{n+1} - \Delta t \left[-\frac{\partial F}{\partial x} + S \right] = 0 \tag{4}$$

where k is the temporal order of accuracy. In the current investigation, both the temporal and spatial accuracy is second order. The time-step size is determined by the Courant-Friedrichs-Lewi condition i.e.

$$\Delta t \le \frac{CFL\ \Delta x}{\left| u_r + c \right|} \tag{5}$$

where *CFL* is the stability number and *c* is the local speed of sound. The CFL stability number for the implicit technique can be very large. Typical values are 100-10,000.

B. Explicit

The explicit time-marching of Eqs. (1) and (2) may also be performed using a Lax-Wendroff scheme, as described by Ni[9]. In this procedure, time-marching the primary variables, *U*, corresponds to an update in time at each node according to a second order temporally accurate Taylor series formula:

$$U_i^{n+1} = U_i^n + \frac{\partial U}{\partial t}\Delta t + \frac{\partial^2 U}{\partial t^2}\frac{\Delta t^2}{2} = U_i^n + \partial U_i + \partial^2 U_i \tag{6}$$

The Ni scheme is a finite volume integration method. The scheme is applied in a three step process. First the *change* is at the center of each computational cell is approximated as

$$\Delta U = \frac{\Delta t}{\Delta x}(F_i^n - F_{i+1}^n) \tag{7}$$

The *correction* to the points *i* and *i+1* are determined using the distribution formulas given below:

$$(\partial U_i) = \frac{1}{2}\left[\Delta U - \frac{\Delta t}{\Delta x}\Delta F \right] \tag{8}$$

$$(\partial U_{i+1}) = \frac{1}{2}\left[\Delta U + \frac{\Delta t}{\Delta x}\Delta F \right] \tag{9}$$

where

$$\Delta F = \left(\frac{\partial F}{\partial U} \right) \Delta U \tag{10}$$

The primary variables are then updated by

$$\partial U_i = (\partial U_i)_{cell_i} + (\partial U_{i+1})_{cell_{i-1}} \tag{11}$$

$$\partial U_i^{n+1} = U_i^n + \partial U_i \tag{12}$$

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The first order changes in time, ∂U, are found directly from application of Eqs. (1) and (2) on the primary computational cells. The second order changes in time, $\partial^2 U$, represented by the second-order derivatives of U above, are found by applying the time-derivative of Eqs. (1) and (2) on computational cells that are translated ½ cell line length from the primary computational cells. The CFL stability number that sets the time-step size is set to 0.7 due to the explicit nature of this scheme.

For steady flows or the inner iteration of the point-implicit technique described below, a multiple-grid acceleration procedure described by Ni is used to greatly reduce the number of time-steps to reach convergence. This allows the scheme to be competitive with the implicit procedure described above.

C. Point Implicit

A point-implicit procedure can be made up from either the implicit or explicit schemes described above. For this procedure, the time-rate changes in Eqs. (4) or (6) are assumed to be in pseudo-time. A true time derivative of the primary variables is added to the right-hand side of Eq. (1). This true time derivative is derived from stored solutions of the primary variables at k+1 previous time-steps, where again, k is the temporal order of accuracy desired. An inner-iteration is then used to drive the right-hand-side to zero. The advantage of this approach is that steady-flow acceleration techniques may be used during the inner iteration such as a multiple-grid scheme. Also, this technique provides flexibility in performing multiple lines of a network in parallel. This procedure is known as the dual-time-step technique[10] and has many similarities to the Newton iteration used in the implicit procedure.

V. Results

Transient pipe flow simulations of gaseous nitrogen and liquid water have been performed to demonstrate the capability of the present procedure. A 0.254 m (10 in) pipe with a 0.0254 m (1 in) diameter was used for these simulations. The surface roughness of the pipe, necessary for viscous flow simulations, was 2.54×10^{-6} m (0.0001 in). The inlet total pressure was held at 3.45 kPa (50 psia) as well as the initial exit static pressure. The inlet total temperature was held at 300°K (540°R). Thus, the initial velocity of the flow in the pipe was zero. At time 0.0001 seconds, the exit pressure was reduced to 3.31 kPa (48 psia). This sudden reduction in pressure initiates a series of expansion and compression waves through the pipe and an increase in the velocity of the flow. For inviscid-flow cases, the pressure decays in the pipe to a uniform value and the velocity grows asymptotically to a uniform value. For viscous-flow cases, the pressure in the pipe decays but to a non-uniform distribution with the inlet pressure higher than the exit due to friction losses. The velocity of the pipe flow, however, will once again grow asymptotically until it reaches a uniform value. All simulations were run in time until both the pressure and velocity distributions through the pipe remained time-independent. A total of 65 grid points with uniform spacing was used along the pipe in order to discretize the governing equations.

A. Transient Nitrogen Pipe Flow

The pipe flow simulation with nitrogen is meant to test the current procedure's capabilities for compressible flow. The explicit and point-implicit numerical procedures were both run in order to make comparisons and to demonstrate features of each technique. Figure 1 shows the predicted pressure and velocity as a function of time using the explicit numerical technique for inviscid flow at five locations along the pipe. In this scheme, the time step size is determined by the minimum time step of all the cells in the domain. The sinusoidal variation of pressure with time is evidence of the expansion and compression waves propagating through the pipe. The time-variation of the velocity corresponds to these waves. The pressure decays in time until it reaches the exit pressure throughout the pipe. The velocity increases until it reaches a value of approximately 31 m/s (102 ft/s).

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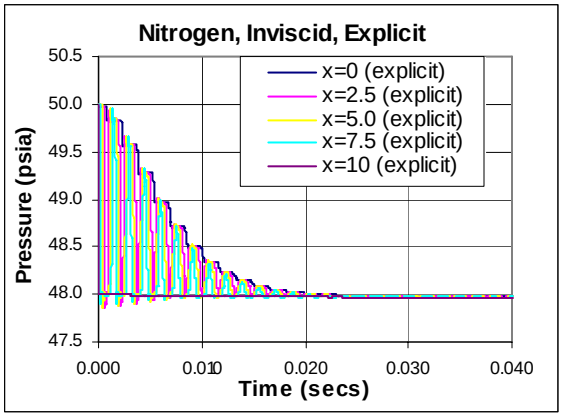
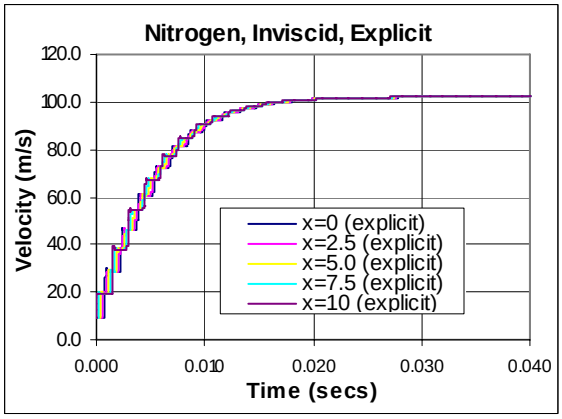
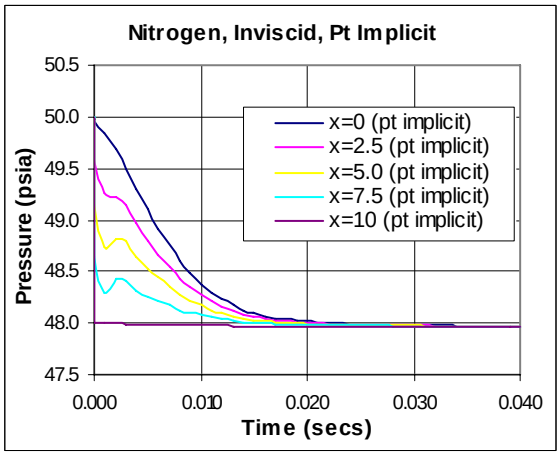


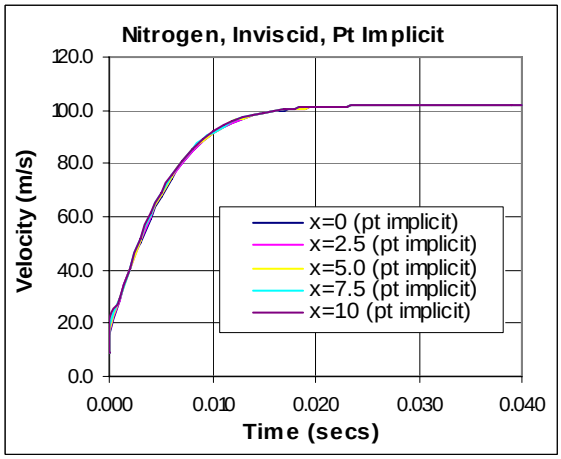


a) Pressure **b) Velocity**

Figure 1 – Nitrogen Transient Inviscid Pipe Flow using Explicit Numerical Technique

Figure 2 shows the predicted results using the point-implicit numerical procedure. In this procedure, the time-step size can be prescribed by the user to be any value that results in a desired solution time and resolution of temporal features in the flow. For the present case, the time-step size was set at 0.01 seconds which was approximately 1,500 times larger than that required for in the explicit procedure. The capability to use a large time-step size in the point-implicit procedure allows for very fast solution time. However, as shown in Figure 2, resolution of the high-frequency waves and their effect on the pressure and velocity is lost as a result of the increased time-step size.





a) Pressure **b) Velocity**

Figure 2 – Nitrogen Transient Inviscid Pipe Flow using Point-Implicit Numerical Technique

Both numerical schemes were run with viscous shear stress effects modeled with a friction factor correlation as described above as a further demonstration of the current procedure's capability. Figure 3 shows the predicted pressure and velocity resulting from the explicit transient viscous flow simulation of nitrogen. The pressure decays to a non-uniform distribution through the pipe for viscous flow. The pressure drop along the pipe agrees very well with what is expected from a lumped parameter analysis with the energy equation. The velocity asymptotically increases with time to a level below that predicted without viscous effects (shown in Figure 1).

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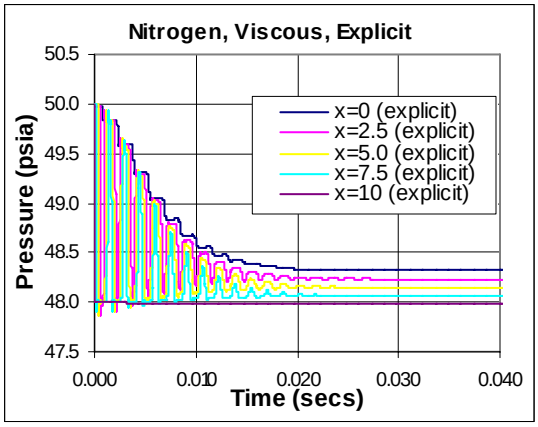
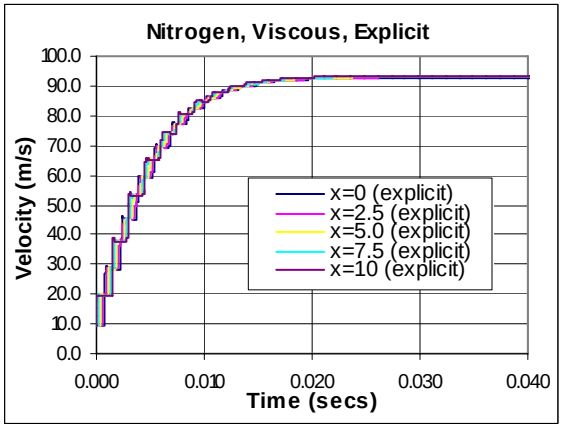
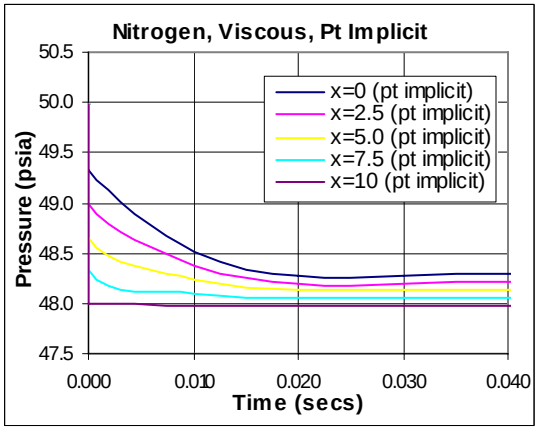


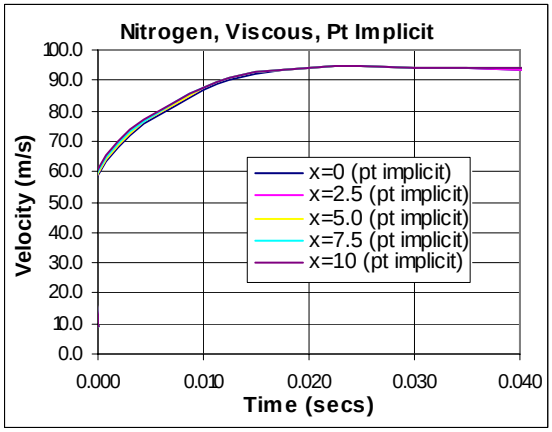


a) Pressure **b) Velocity**

Figure 3 – Nitrogen Transient Viscous Pipe Flow using Explicit Numerical Technique

The nitrogen viscous flow results using the point-implicit numerical procedure are shown in Figure 4. The transient solution is obtained with a time-step size 1,500 times greater than that for the explicit solution shown in Figure 3 but with the loss in temporal resolution of the pressure and velocity solution.





a) Pressure **b) Velocity**

Figure 4 – Nitrogen Transient Viscous Pipe Flow using Point-Implicit Numerical Technique

Transient Water Pipe Flow

A similar set of simulations were performed using the present procedure with water to demonstrate the capability to predict transient flows in incompressible fluids. The main critical difference with incompressible fluids is that the speed of sound and wave speeds are much larger for incompressible fluids. This makes the use of explicit numerical techniques time-consuming. Resolution of the unsteady sinusoidal transients shown above are possible, but quite time consuming. The effect of the high-frequency waves are not always of interest so that numerical techniques that can take large time-steps and reduce solution time are often attractable.

Figure 5 shows the transient point-implicit inviscid solution of water through the previously described configuration. Note that the time to reach equilibrium for water is much longer than that required for nitrogen due to the incompressibility of the fluid.

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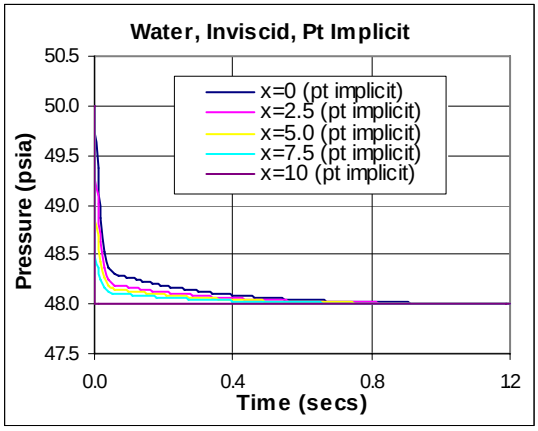
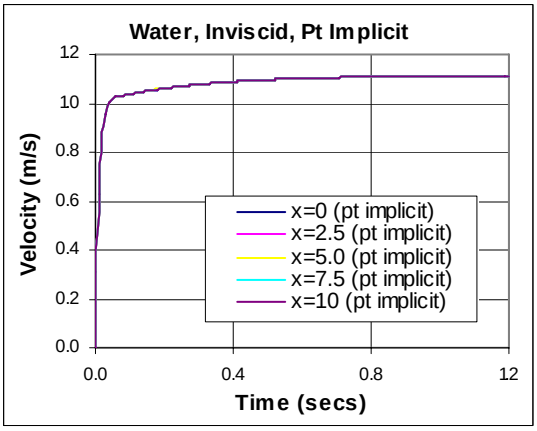


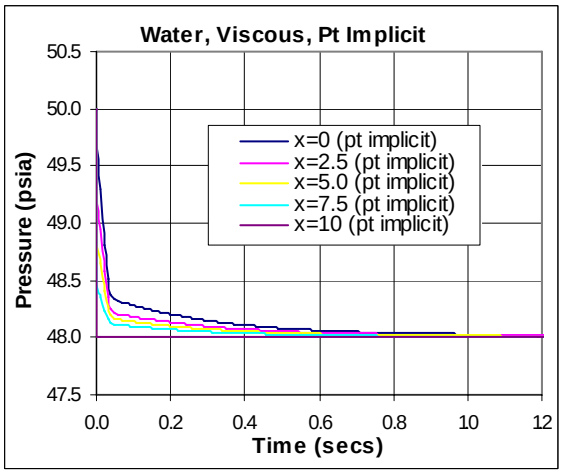


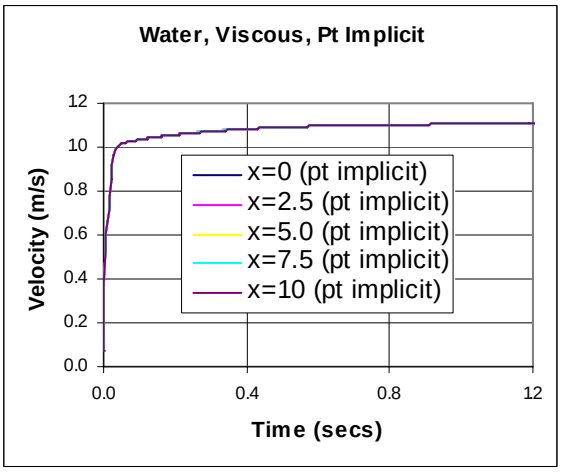
a) Pressure **b) Velocity**

Figure 5 – Water Transient Inviscid Pipe Flow using Point-Implicit Numerical Technique

The size of the time step used in the point-implicit solution was 0.01 seconds. The time step size required in the corresponding explicit solution procedure was approximately 2×10^{-6} seconds or 5,000 times smaller than that used in the point-implicit solution. As a result, over 600,000 time steps would be required to solve the 1.2 seconds of time to reach a time-independent solution.

The transient viscous solution for water pipe flow using the point-implicit procedure is shown in Figure 6. The viscous pressure solution converges to a non-uniform time-independent distribution that agrees very well with lumped parameter energy equation analysis. The velocity converges to a uniform time-independent solution with a slightly lower velocity than the predicted inviscid time-independent solution.





a) Pressure **b) Velocity**

Figure 6 – Water Transient Viscous Pipe Flow using Point-Implicit Numerical Technique

As for the inviscid case, the time step size required for the explicit solution is approximately 5,000 times smaller requiring an excessive solution time. Both inviscid and viscous solutions have been run, however, to verify solution capability. Comparison between the explicit and point-implicit solutions are similar to that for nitrogen with the explicit solutions showing very high frequency content due to the various expansion and compression waves propagating through the pipe.

VI. Conclusion

A new baseline procedure has been developed for the numerical solution of transient quasi two-dimensional flow in engine and system lines and volumes. This new procedure is driven written in both Matlab/Simulink and

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Fortran95. A variety of numerical solution algorithms are included to allow for various needs depending on the desired solution time and frequency resolution. Currently, explicit and point-implicit numerical techniques have been implemented and validated. The point-implict technique is very useful for finding rapid turn-around of solutions at the expense of some loss in temporal resolution. The explicit technique is very useful for predicting the high-frequency content of transient flow fields. Implementation of a fully implicit numerical technique is underway and results will also be shown for this technique in the final paper.

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